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On the uniqueness of Euclidean distance matrix completions

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Abstract

The Euclidean distance matrix completion problem (EDMCP) is the problem of determining whether or not a given partial matrix can be completed into a Euclidean distance matrix. In this paper, we present necessary and sufficient conditions for a given solution of the EDMCP to be unique.

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1. Introduction

All matrices considered in this paper are real. An $n \times n$ matrix $D = (d_{ij})$ is said to be a *Euclidean distance matrix* (EDM) iff there exist points $p^1, p^2, \ldots, p^n$ in some Euclidean space such that $d_{ij} = \|p^i - p^j\|^2$ for all $i, j = 1, \ldots, n$. It immediately follows that if D is EDM then D is symmetric with positive entries and with zero diagonal. We say matrix $A = (a_{ij})$ is *symmetric partial* if only some of its entries are specified and a_{ji} is specified and equal to a_{ij} whenever a_{ij} is specified. The unspecified entries of A are said to be *free*. Given an $n \times n$ symmetric partial matrix A, an $n \times n$ matrix D is said to be a *EDM completion* of A iff D is EDM and

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$d_{ij} = a_{ij}$ for all specified entries of A. The *Euclidean distance matrix completion problem* (EDMCP) is the problem of determining whether or not there exists an EDM completion for a given symmetric partial matrix A. To avoid trivialities, we always assume that the diagonal entries of A are specified and equal to zero; and all specified off-diagonal entries of A are positive.

Applications of EDMs and the EDMCP include among others, molecular conformation theory, protein folding, and the statistical theory of multidimensional scaling [5,11,16]. As a result, EDMs and the EDMCP have received a lot of attention in the literature. For characterization and properties of EDMs see [6,8,10,19]. Theoretical properties including graph theoretic conditions for existence of EDM completions can be found in [4,12,13,15]. A classic paper on the closely related positive semidefinite matrix completion problem is [9]. Algorithmic aspects of the EDMCP are discussed in [3,17,20]. For a recent survey see [14].

Let A be a symmetric partial matrix and let D be a given EDM completion of A. Such D can be obtained, for example, by using the algorithm discussed in [3]. In this paper, we present necessary and sufficient conditions for D to be unique. These conditions are given in terms of Gale transforms of the points p^i that generate D.

1.1. Notation

We denote by $\mathscr{S}_n$ the space of $n \times n$ symmetric matrices. The inner product on $\mathscr{S}_n$ is given by

$$\langle A, B\rangle := \operatorname{trace}(AB).$$

Positive semidefiniteness (positive definiteness) of a symmetric matrix A is denoted by $A \succeq 0$ ($A \succ 0$). We denote by e the vector, of the appropriate dimension, of all ones; and by E^{ij} the symmetric matrix, of the appropriate dimension, with ones in the (i, j)th and (j, i)th entries and zeros elsewhere. The $n \times n$ identity matrix will be denoted by I_n. $A \circ B$ denotes the *Hadamard* i.e., the element-wise product of matrices A and B. The diagonal of a matrix A will be denoted by diag A. Finally, the null space of a matrix X is denoted by $\mathscr{N}(X)$.

2. Preliminaries

It is well known [6,8,19] that a symmetric $n \times n$ matrix D with zero diagonal is EDM if and only if D is negative semidefinite on the subspace

$$M := \{x \in \Re^n : e^{\mathrm{T}}x = 0\}.$$

Let V be an $n \times (n-1)$ matrix whose columns form an orthonormal basis of M; that is, V satisfies:

$$V^{\mathrm{T}}e = 0, \quad V^{\mathrm{T}}V = I_{n-1}. \tag{1}$$

Then the orthogonal projection on M, denoted by J, is given by $J := VV^{\mathrm{T}} = I - ee^{\mathrm{T}}/n$. Hence, it follows that if D is a symmetric matrix with zero diagonal then

$$D \text{ is EDM iff } B = \mathscr{T}(D) := -\frac{1}{2} JDJ \succeq 0. \tag{2}$$

Let rank $B = r$. Then the points $p^1, p^2, \ldots, p^n$ that generate D are given by the rows of the $n \times r$ matrix P where $B := PP^{\mathrm{T}}$. P is called *a realization* of D in $\Re^r$. Note that the centroid of the points p^i, $i = 1, \ldots, n$ coincides with the origin since $Be = 0$.

Let D be EDM and let

$$P := \begin{bmatrix} p^{1^{\mathrm{T}}} \\ p^{2^{\mathrm{T}}} \\ \vdots \\ p^{n^{\mathrm{T}}} \end{bmatrix}$$

be a realization of D in $\Re^r$. Assume that the points $p^1, p^2, \ldots, p^n$ are not contained in a proper hyperplane. Then $P^{\mathrm{T}}e = 0$ and rank $P = r$. Let $\bar{r} = n - 1 - r$. For $\bar{r} \geqslant 1$, let Λ be an $n \times \bar{r}$ matrix, whose columns form a basis for the null space of the $(r + 1) \times n$ matrix

$$\begin{bmatrix} P^{\mathrm{T}} \\ e^{\mathrm{T}} \end{bmatrix};$$

i.e.,

$$P^{\mathrm{T}}\Lambda = 0, \quad e^{\mathrm{T}}\Lambda = 0, \quad \text{and} \quad \Lambda \text{ has full column rank.} \tag{3}$$

Λ is called a *Gale matrix* corresponding to D; and the ith row of Λ, considered as a vector in $\Re^{\bar{r}}$, is called a Gale transform of p^i [7]. Gale transform is a well-known technique used in the theory of polytopes. Three remarks are in order here. First, the entries of Λ are rational whenever the entries of P are rational. Second, the columns of Λ represent the affine dependence relations among the points $p^1, p^2, \ldots, p^n$, i.e., among the rows of P. Third, Λ is not unique. In fact, for any non-singular $\bar{r} \times \bar{r}$ matrix Q, ΛQ satisfies (3); hence, ΛQ is also a Gale matrix. We will exploit this property to define a special Gale matrix Z which is more sparse than Λ and more convenient for the purposes of this paper.

Let us write Λ in block form as

$$\Lambda = \begin{bmatrix} \Lambda_1 \\ \Lambda_2 \end{bmatrix},$$

where Λ_1 is $\bar{r} \times \bar{r}$ and Λ_2 is $(r + 1) \times \bar{r}$. By relabeling the points $p^1, p^2, \ldots, p^n$, if necessary, we can assume without loss of generality that Λ_1 is non-singular. Then Z is defined as

$$Z := \Lambda\Lambda_1^{-1} = \begin{bmatrix} I_{\bar{r}} \\ \Lambda_2\Lambda_1^{-1} \end{bmatrix}. \tag{4}$$

Let $z^{i^{\mathrm{T}}}$ denote the ith row of Z; i.e.,

$$Z := \begin{bmatrix} z^{1^{\mathrm{T}}} \\ z^{2^{\mathrm{T}}} \\ \vdots \\ z^{n^{\mathrm{T}}} \end{bmatrix}.$$

Hence, z^i, the Gale transforms of p^i, for $i = 1, \ldots, \bar{r}$ is equal to the ith unit vector in $\Re^{\bar{r}}$.

2.1. The set of EDM completions

In this section we characterize the set of EDM completions of a symmetric partial matrix A given one EDM completion D_1. As we remarked earlier, such D_1 can be obtained using, for example, the algorithm presented in [3]. This set of EDM completions was first characterized in [1] in the context of realizations of weighted graphs in Euclidean spaces. For completeness we present, next, the details of this characterization.

It would be more convenient for the purposes of this paper to use the following characterization of EDMs which is equivalent to (2). Let D be an $n \times n$ symmetric matrix with zero diagonal. Then

$$D \text{ is EDM iff } X = \mathscr{T}_V(D) := -\tfrac{1}{2}V^{\mathrm{T}}DV \succeq 0. \tag{5}$$

Note that $X \in \mathscr{S}_{n-1}$. It is not difficult to show that

$$D = \mathscr{K}_V(X) := \operatorname{diag}(VXV^{\mathrm{T}})e^{\mathrm{T}} + e\operatorname{diag}(VXV^{\mathrm{T}})^{\mathrm{T}} - 2VXV^{\mathrm{T}}. \tag{6}$$

For a proof of (5) and (6) see [3]. Let D_1 be an EDM completion of a given symmetric partial matrix A and let $X_1 = \mathscr{T}_V(D_1)$ and $B_1 = \mathscr{T}(D_1)$. Then (1) and (2) imply that $B_1 = VX_1V^{\mathrm{T}}$ and $X_1 = V^{\mathrm{T}}B_1V$. Hence, D_1, B_1 and X_1 uniquely determine each other. Note that $\operatorname{rank} X_1 = \operatorname{rank} B_1 = \operatorname{rank} P$ where $B_1 = PP^{\mathrm{T}}$.

Let $H = (h_{ij})$ be the 0–1 matrix where $h_{ij} = 1$ if a_{ij} is specified and $h_{ij} = 0$ if a_{ij} is free. Let $2\bar{m}$ be the number of free entries in A. Recall that we always assume that diag A is specified and equal to 0. Also we assume that A has at least two free entries, i.e., $\bar{m} \geqslant 1$. Define the linear operator

$$\mathscr{A}(X) := H \circ \mathscr{K}_V(X), \tag{7}$$

where $\circ$ denotes the Hadamard product. Let D be any EDM completion of A. Then $X = \mathscr{T}_V(D) \succeq 0$ and $H \circ \mathscr{K}_V(X) = H \circ \mathscr{K}_V(X_1) = H \circ D_1$; that is, $(X - X_1) \in \mathscr{N}(\mathscr{A})$. This follows since d_{ij} can differ from d_{1ij} only if a_{ij} is free; i.e., $h_{ij} = 0$.

Let $E^{ij} \in \mathscr{S}_n$ be the matrix with ones in the (i, j)th and the (j, i)th entries and zeros elsewhere. For each free entry a_{ij} and $i < j$, define the matrices M^k, $k = 1, \ldots, \bar{m}$, such that

$$M^k := -\tfrac{1}{2} V^{\mathrm{T}} E^{ij} V. \tag{8}$$

Then it is easy to show that $\{M^k : k = 1, \dots, \bar{m}\}$ is a set of linearly independent matrices, and that $\{M^k : k = 1, \dots, \bar{m}\}$ forms a basis for $\mathscr{N}(\mathscr{A})$. Thus,

$$\mathscr{N}(\mathscr{A}) = \left\{ B \in \mathscr{S}_{n-1} : B = \sum_{k=1}^{\bar{m}} y_k M^k \ \text{ for some } \ y \in \Re^{\bar{m}} \right\}. \tag{9}$$

Therefore, the set of EDM completions is given by the following theorem.

Theorem 2.1 [1]. *Given D_1, an EDM completion of a given symmetric partial matrix A, let*

$$\Omega := \left\{ y \in \Re^{\bar{m}} : X(y) := X_1 + \sum_{k=1}^{\bar{m}} y_k M^k \succeq 0 \right\}, \tag{10}$$

where $X_1 = \mathscr{T}_V(D_1) = -\frac{1}{2} V^{\mathrm{T}} D_1 V$. Then, $\{D : D = \mathscr{K}_V(X(y)),\ y \in \Omega\}$ is the set of all EDM completions of A.

Let $\mathscr{P}_{n-1}$ denote the cone of positive semidefinite matrices of order $n-1$. Then clearly

$$\{X(y) : y \in \Omega\} = (X_1 + \mathscr{N}(\mathscr{A})) \cap \mathscr{P}_{n-1}.$$

Note that Ω is a closed, convex, and generally non-polyhedral set. Since $X_1 \succeq 0$, the origin is always contained in Ω. For more on the properties of Ω see [1]. Therefore, D_1 is unique if and only if Ω is a singleton set; that is, $\Omega = \{0\}$.

3. Main results

In this section we present the main results of the paper. Recall that if D_1 is EDM then $X_1 = \mathscr{T}_V(D_1) = -\frac{1}{2} V^{\mathrm{T}} D_1 V$ is a positive $(n-1) \times (n-1)$ matrix. First we consider the case where X_1 is non-singular.

Theorem 3.1. *Given a partial symmetric matrix A, let D_1 be an EDM completion of A and let $X_1 = \mathscr{T}_V(D_1)$. If X_1 is non-singular, i.e.,* rank $X_1 = n-1$, *then D_1 is not unique.*

Proof. If rank $X_1 = n-1$, then $X_1 \succ 0$. Let y be any non-zero vector in $\Re^{\bar{m}}$, then $X(y/\lambda) = X_1 + \sum_{k=1}^{\bar{m}} y_k/\lambda M^k \succeq 0$ for sufficiently large positive scalar λ. Hence, $y/\lambda \in \Omega$ and the result follows. $\square$

Theorem 3.1 has a simple geometrical interpretation. If X_1 is non-singular. Then X_1 is in the interior of $\mathscr{P}_{n-1}$, the positive semidefinite cone of order $n-1$. Hence, one can move a little bit in any direction taken from the null space of $\mathscr{A}$ and stay within $\mathscr{P}_{n-1}$. Therefore, in this case Ω is not a singleton. If X_1 is singular then the following theorem holds.

Theorem 3.2. *Given a partial symmetric matrix* A, *let* D_1 *be an EDM completion of* A *and let* $X_1 = \mathscr{T}_V(D_1)$. *If* X_1 *is singular, i.e.,* $\bar{r} = n - 1 - \operatorname{rank} X_1 \geqslant 1$, *let* U *be an* $(n-1) \times \bar{r}$ *matrix whose columns form an orthonormal basis for* $\mathscr{N}(X_1)$. *Then the following is a sufficient condition for* Ω *to be a singleton; i.e.,* $\Omega = \{0\}$:

$$\exists\, \bar{r} \times \bar{r} \ \text{matrix} \ \Psi \succ 0 \ \text{such that} \ \langle U \Psi U^{\mathrm{T}}, M^k \rangle = 0 \quad \text{for} \ k = 1, \ldots, \bar{m}. \tag{11}$$

Condition (11) *is also necessary if the following condition holds*:

$$\operatorname{rank}(U^{\mathrm{T}} \mathscr{M}(\hat{y}) U) = \operatorname{rank}(\mathscr{M}(\hat{y}) U), \tag{12}$$

where $\mathscr{M}(\hat{y}) = \sum_{k=1}^{\bar{m}} \hat{y}_k M^k$ *for some* $\hat{y} \in \Re^{\bar{m}}$, $\hat{y} \neq 0$, *such that* $U^{\mathrm{T}} \mathscr{M}(\hat{y}) U$ *is non-zero positive semidefinite.*

The proof of Theorem 3.2, which uses the notion of polarity in convexity theory, is given in Section 4. A comment is in order here. As will be shown in Corollary 4.2, there always exists a $\hat{y} \in \Re^{\bar{m}}$, $\hat{y} \neq 0$, such that $U^{\mathrm{T}} \mathscr{M}(\hat{y}) U$ is non-zero positive semidefinite whenever condition (11) fails to hold. However, $\operatorname{rank}(U^{\mathrm{T}} \mathscr{M}(\hat{y}) U)$ may or may not be equal to $\operatorname{rank}(\mathscr{M}(\hat{y}) U)$. A case where $\operatorname{rank}(U^{\mathrm{T}} \mathscr{M}(\hat{y}) U) = \operatorname{rank}(\mathscr{M}(\hat{y}) U)$ is given in the next corollary.

Corollary 3.1. *If* $\operatorname{rank} X_1 = n - 2$. *Then condition* (11) *is both necessary and sufficient for* Ω *to be a singleton.*

Proof. If condition (11) fails to hold, then by Corollary 4.2, there exists a $\hat{y} \in \Re^{\bar{m}}$ such that $U^{\mathrm{T}} \mathscr{M}(\hat{y}) U$ is non-zero positive semidefinite. If $\operatorname{rank} X_1 = n - 2$ then $\bar{r} = 1$. This implies that $U^{\mathrm{T}} \mathscr{M}(\hat{y}) U$ is a positive scalar. Thus, $\operatorname{rank} U^{\mathrm{T}} \mathscr{M}(\hat{y}) U = \operatorname{rank} \mathscr{M}(\hat{y}) U$ trivially holds and the result follows. □

The next theorem is the main result of the paper. It is given in terms of Gale transforms of points $p^1, p^2, \ldots, p^n$ that generate D_1; and it follows directly from Theorems 2.1, 3.1 and 3.2 and Corollary 3.1.

Theorem 3.3. *Let* A *be a given partial symmetric matrix and let* D_1 *be an EDM completion of* A. *Let* $X_1 = \mathscr{T}_V(D_1)$ *and let* $\bar{r}$ *be the nullity of* X_1, *i.e.,* $\bar{r} = n - 1 - \operatorname{rank} X_1$. *Then*:

1. *If* $\bar{r} = 0$, *then* D_1 *is not unique.*
2. *If* $\bar{r} \geqslant 1$, *let* Z *be the Gale matrix corresponding to* D_1 *defined in* (4). *Then*
   (a) *If* $\bar{r} = 1$, *then the following condition is necessary and sufficient for* D_1 *to be unique*:
      (i) *There exists a positive definite* $\bar{r} \times \bar{r}$ *matrix* Ψ *such that* $z^{i^{\mathrm{T}}} \Psi z^j = 0$ *for all* i, j *such that* a_{ij} *is free.*
   (b) *If* $\bar{r} \geqslant 2$, *then condition* (i) *is sufficient for* D_1 *to be unique. Condition* (i) *is also necessary if the following condition holds*:

$$\operatorname{rank} \mathscr{Z}(\hat{y}) = \operatorname{rank}(V^{\mathrm{T}} \mathscr{E}(\hat{y}) Z), \tag{13}$$

where $\mathscr{Z}(\hat{y}) = \sum_{k=1}^{\bar{m}} \hat{y}_k (z^i z^{j^{\mathrm{T}}} + z^j z^{i^{\mathrm{T}}})$ *and* $\mathscr{E}(\hat{y}) = \sum_{k=1}^{\bar{m}} \hat{y}_k E^{ij}$ *for some* $\hat{y} \in \Re^{\bar{m}}$, $\hat{y} \neq 0$, *such that* $\mathscr{Z}(\hat{y})$ *is non-zero positive semidefinite.*

Two comments are in order here. First, in Example 2, it will be shown that condition (13) is essential to ensure the necessity of condition (i) in Theorem 3.3. Thus the *gap* between sufficiency and necessity in Theorem 3.3 can not be closed. Second, it is of great interest to investigate the problem of devising an algorithm for checking whether or not a given EDM completion is unique using the characterization presented in Theorem 3.3. Such an investigation will be the subject of a future paper.

Before proving Theorem 3.3, we present the following lemmas establishing the relationship between the matrices U and M^k in Theorem 3.2 and the Gale matrix Z.

Lemma 3.1. *Let* D_1 *be a EDM and let* $X_1 = \mathscr{T}_V(D_1)$ *as defined in* (5). *Then*

$$\mathscr{N}(X_1) = \mathscr{N}(P^{\mathrm{T}} V),$$

where P *is a realization of* D_1.

Proof. Since $B_1 = \mathscr{T}(D_1) = PP^{\mathrm{T}}$, we have $\mathscr{N}(X_1) = \mathscr{N}(V^{\mathrm{T}} B_1 V) = \mathscr{N}(V^{\mathrm{T}} P P^{\mathrm{T}} V) = \mathscr{N}(P^{\mathrm{T}} V)$. □

The following lemma was first proved in [2]. We include the proof here for completeness.

Lemma 3.2. *Let* D_1 *be a EDM and let* U *be the matrix whose columns form an orthonormal basis of the null space of* $X_1 = \mathscr{T}_V(D_1)$. *Then* VU *is a Gale matrix*; *i.e.*, $VU = ZQ$ *for some non-singular matrix* Q.

Proof. It follows from Lemma 3.1 that $P^{\mathrm{T}} VU = X_1 U = 0$ and from the definition of V in (1) that $e^{\mathrm{T}} VU = 0$. Hence, the columns of VU form an orthonormal basis for the null space of

$$\begin{bmatrix} P^{\mathrm{T}} \\ e^{\mathrm{T}} \end{bmatrix}.$$

Hence, VU is a Gale matrix and the result follows. □

Proof of Theorem 3.3. That $\langle U\Psi U^{\mathrm{T}}, M^k\rangle = -\frac{1}{2}\langle \Psi, U^{\mathrm{T}}V^{\mathrm{T}}E^{ij}VU\rangle = -\frac{1}{2}\langle Q\Psi Q^{\mathrm{T}}, Z^{\mathrm{T}}E^{ij}Z\rangle$ follows directly from (8) and Lemma 3.2. Hence, condition (11) is equivalent to condition (i) in the theorem since Q is non-singular. Furthermore, condition (12) is equivalent to condition (13) since $\mathrm{rank}(U^{\mathrm{T}}\mathscr{M}(\hat{y})U) = \mathrm{rank}\,\mathscr{X}(\hat{y})$ and $\mathrm{rank}(\mathscr{M}(\hat{y})U) = \mathrm{rank}(V^{\mathrm{T}}\mathscr{E}(\hat{y})Z)$. $\square$

4. Proof of Theorem 3.2

Let K be a cone in $\mathscr{S}_n$, we denote the closure of K and the interior of K by $\mathrm{cl}\,K$ and $\mathrm{int}(K)$ respectively. The *polar* of K, denoted by K°, is defined as

$$K^\circ = \{C \in \mathscr{S}_n : \langle C, X\rangle \leqslant 0 \text{ for all } X \in K\}.$$

Then it immediately follows that K° is always a convex closed cone. The following facts are well known [18].

Lemma 4.1. *Let K be a cone in $\mathscr{S}_n$ and let $\mathscr{L}$ be a subspace of $\mathscr{S}_n$. Then*:

1. $(K^\circ)^\circ = \mathrm{cl}\,K$,
2. $(\mathrm{int}(K))^\circ = K^\circ$,
3. $\mathscr{L}^\circ = \mathscr{L}^\perp$, *where $\mathscr{L}^\perp$ is the orthogonal complement of $\mathscr{L}$.*

Let $\mathscr{P}_{n-1}$ denote the cone of positive semidefinite matrices in $\mathscr{S}_{n-1}$; i.e., $\mathscr{P}_{n-1} = \{A \in \mathscr{S}_{n-1} : A \succeq 0\}$. Then it is also well known [21] that $\mathscr{P}_{n-1}$ is closed and $\mathscr{P}_{n-1}^\circ = -\mathscr{P}_{n-1}$.

Let $R(\mathscr{P}_{n-1}, X_1)$ and $N(\mathscr{P}_{n-1}, X_1)$ denote respectively the *radial cone* and the *normal cone* of $\mathscr{P}_{n-1}$ at X_1; that is,

$$\begin{aligned} R(\mathscr{P}_{n-1}, X_1) &= \{A \in \mathscr{S}_{n-1} : A = \lambda(X - X_1), \lambda \geqslant 0, X \succeq 0\}, \\ N(\mathscr{P}_{n-1}, X_1) &= \{C \in \mathscr{S}_{n-1} : \langle C, X_1\rangle \geqslant \langle C, X\rangle, \forall X \succeq 0\}. \end{aligned} \tag{14}$$

Then it immediately follows that

$$\begin{aligned} N(\mathscr{P}_{n-1}, X_1) &= (R(\mathscr{P}_{n-1}, X_1))^\circ, \\ (N(\mathscr{P}_{n-1}, X_{n-1}))^\circ &= \mathrm{cl}\,R(\mathscr{P}_{n-1}, X_1) = T(\mathscr{P}_{n-1}, X_1), \end{aligned} \tag{15}$$

where $T(\mathscr{P}_{n-1}, X_1)$ is called the *tangent cone* of $\mathscr{P}_{n-1}$ at X_1. The following is a technical lemma.

Lemma 4.2. *Let $A \succeq 0$, and $Y \succeq 0$ and let $\langle A, Y\rangle = 0$. Then $Y = U\Psi U^{\mathrm{T}}$ for some $\Psi \succeq 0$ where U is the matrix whose columns form an orthonormal basis for the null space of A.*

Proof. Let W be the matrix whose columns form an orthonormal basis for the range space of A and let U be the matrix whose columns form an orthonormal basis for the null space of A. Thus the matrix $Q = [W \quad U]$ is orthogonal. Since both A and Y are positive semidefinite, it is well known that $\langle A, Y\rangle = 0$ if and only if $AY = 0$. But $AY = 0$ implies that $\mathrm{diag}(W^{\mathrm{T}}YW) = 0$, and since $W^{\mathrm{T}}YW \succeq 0$, it also implies that $W^{\mathrm{T}}YW = 0$. Furthermore, since

$$Q^{\mathrm{T}}YQ = \begin{bmatrix} W^{\mathrm{T}}YW & W^{\mathrm{T}}YU \\ U^{\mathrm{T}}YW & U^{\mathrm{T}}YU \end{bmatrix} \succeq 0,$$

it follows that $W^{\mathrm{T}}YU = U^{\mathrm{T}}YW = 0$. Let $\Psi = U^{\mathrm{T}}YU$, then

$$Y = [W \quad U]\begin{bmatrix} 0 & 0 \\ 0 & \Psi \end{bmatrix}\begin{bmatrix} W^{\mathrm{T}} \\ U^{\mathrm{T}} \end{bmatrix} = U\Psi U^{\mathrm{T}}. \qquad \square$$

The next lemma gives a characterization of the normal cone and the tangent cone of $\mathscr{P}_{n-1}$ at X_1.

Lemma 4.3. *Let U be the matrix whose columns form an orthonormal basis for $\mathscr{N}(X_1)$. Then*

$$\begin{aligned} &1.\ N(\mathscr{P}_{n-1}, X_1) = \left\{C \in \mathscr{S}_{n-1} : C = -U\Psi U^{\mathrm{T}} \text{ for all } \Psi \succeq 0\right\}, \\ &2.\ T(\mathscr{P}_{n-1}, X_1) = \left\{A \in \mathscr{S}_{n-1} : U^{\mathrm{T}}AU \succeq 0\right\}. \end{aligned} \tag{16}$$

Proof. (1) Let $C = -U\Psi U^{\mathrm{T}}$ for some $\Psi \succeq 0$. Then $\langle C, X_1 - X\rangle = \langle \Psi, U^{\mathrm{T}}XU\rangle \geqslant 0$ for all $X \succeq 0$. Hence, $C \in N(\mathscr{P}_{n-1}, X_1)$. On the other hand, let $C \in N(\mathscr{P}_{n-1}, X_1)$ and consider the following semidefinite program

$$\text{(P)} \quad \mu = \max_X \left\{\langle C, X\rangle : X \succeq 0\right\}.$$

Then by the definition of $N(\mathscr{P}_{n-1}, X_1)$ it follows that $\mu = \langle C, X_1\rangle$. Now the dual semidefinite program is

$$\text{(D)} \quad \nu = \min_Y \left\{\langle 0, Y\rangle : Y = -C \text{ and } Y \succeq 0\right\}.$$

Since Slater's constraint qualification (i.e., the set of feasible solutions of (P) contains an $X \succ 0$) trivially holds for (P) (see e.g. [21]), by strong duality of semidefinite programming it follows that $C = -Y$, $\langle C, X_1\rangle = 0$ for some $Y \succeq 0$. Using Lemma 4.2 we have $C = -U\Psi U^{\mathrm{T}}$ for some $\Psi \succeq 0$.

(2) Follows immediately form part 1 and the definition of polar cone. $\square$

Lemma 4.4. *Let $\mathscr{L} = \{A \in \mathscr{S}_{n-1} : A = \sum_{k=1}^{\bar{m}} y_k M^k$ for some $y \in \Re^{\bar{m}}\}$, where M^k are defined in* (8). *Then*

$$\Omega = \{0\} \quad \textit{if and only if} \quad \mathscr{L} \cap R(\mathscr{P}_{n-1}, X_1) = \{0\}.$$

Proof. Let $\Omega = \{0\}$ and assume that $A \in \mathscr{L} \cap R(\mathscr{P}_{n-1}, X_1)$ and $A \neq 0$. Then there exists $y \in \Re^{\bar{m}}$, $y \neq 0$ and $\lambda > 0$, $X \succeq 0$, $X \neq X_1$ such that $A = \sum_{k=1}^{\bar{m}} y_k M^k = \lambda(X - X_1)$. Therefore, $X_1 + \sum_{k=1}^{\bar{m}} y_k/\lambda M^k \succeq 0$. Hence $y/\lambda \in \Omega$, a contradiction.

On the other hand, let $\mathscr{L} \cap R(\mathscr{P}_{n-1}, X_1) = \{0\}$ and assume that there exists $y \in \Omega$, $y \neq 0$. Therefore $X = X_1 + \sum_{k=1}^{\bar{m}} y_k M^k \succeq 0$. Hence, $A = \sum_{k=1}^{\bar{m}} y_k M^k = X - X_1 \neq 0$ and $A \in \mathscr{L} \cap R(\mathscr{P}, X_1)$, a contradiction. □

Note that Theorem 3.1 follows also from Lemma 4.4 since if $X_1 \succ 0$ then $R(\mathscr{P}_{n-1}, X_1) = \mathscr{S}_{n-1}$, hence $\mathscr{L} \cap R(\mathscr{P}_{n-1}, X_1) = \mathscr{L}$.

Lemma 4.5. *Let K be a cone in $\mathscr{S}_{n-1}$ and let $\mathscr{L}$ be a subspace of $\mathscr{S}_{n-1}$. Then*

$$\mathscr{L}^{\perp} \cap \operatorname{int}(K^{\circ}) \neq \emptyset \quad \textit{if and only if} \quad \mathscr{L} \cap \operatorname{cl} K = \{0\}.$$

Proof. Let $A \in \mathscr{L}^{\perp} \cap \operatorname{int}(K^{\circ})$ and assume that there exists a non-zero matrix $C \in \mathscr{L} \cap \operatorname{cl} K$. Then $\langle A, C\rangle = 0$ since $A \in \mathscr{L}^{\perp}$ and $C \in \mathscr{L}$. On the other hand, $\langle A, C\rangle < 0$ since $A \in \operatorname{int}(K^{\circ})$ and $C \neq 0$, $C \in \operatorname{cl} K = (\operatorname{int}(K^{\circ}))^{\circ}$; hence a contradiction.

Now Let $\mathscr{L}^{\perp} \cap \operatorname{int}(K^{\circ}) = \emptyset$, then by the separation theorem [18] there exists $Y \neq 0$ such that $\langle Y, A\rangle = 0$ for all $A \in \mathscr{L}^{\perp}$ and $\langle Y, C\rangle \leqslant 0$ for all $C \in \operatorname{int}(K^{\circ})$. Therefore, $Y \in \mathscr{L}$ and $Y \in (\operatorname{int}(K^{\circ}))^{\circ} = (K^{\circ})^{\circ}$, hence $Y \in \mathscr{L} \cap \operatorname{cl} K$ and the result follows. □

Corollary 4.1. *If condition* (11) *in Theorem* 3.2 *holds then $\Omega = \{0\}$.*

Proof. Follows from Lemma 4.5 by setting $\mathscr{L} = \{A \in \mathscr{S}_{n-1} : A = \sum_{k=1}^{\bar{m}} \hat{y}_k M^k$, $y \in \Re^{\bar{m}}\}$ and $K = R(\mathscr{P}_{n-1}, X_1)$ since $\mathscr{L} \cap \operatorname{cl} K = \{0\}$ implies that $\mathscr{L} \cap K = \{0\}$. □

Corollary 4.2. *Condition* (11) *in Theorem* 3.2 *fails to hold if and only if there exists $\hat{y} \in \Re^{\bar{m}}$, $\hat{y} \neq 0$ such that*

$$U^{\mathrm{T}} \mathscr{M}(\hat{y}) U \quad \textit{is non-zero positive semidefinite},$$

where $\mathscr{M}(\hat{y}) = \sum_{k=1}^{\bar{m}} \hat{y}_k M^k$.

Proof. Follows from Lemma 4.5 by setting $\mathscr{L} = \{A \in \mathscr{S}_{\bar{r}} : A = \sum_{k=1}^{\bar{m}} \hat{y}_k U^{\mathrm{T}} M^k U$, $y \in \Re^{\bar{m}}\}$ and $K = \mathscr{P}_{\bar{r}}$ since $\mathscr{P}_{\bar{r}}$ is closed and $\mathscr{P}_{\bar{r}}{}^{\circ} = -\mathscr{P}_{\bar{r}}$. □

Lemma 4.6. *Let there exists $\hat{y} \in \Re^{\bar{m}}$, $\hat{y} \neq 0$ such that*

$$U^{\mathrm{T}} \mathscr{M}(\hat{y}) U \quad \textit{is non-zero positive semidefinite},$$

where $\mathscr{M}(\hat{y}) = \sum_{k=1}^{\bar{m}} \hat{y}_k M^k$. If $\mathscr{N}(U^{\mathrm{T}} \mathscr{M}(\hat{y}) U) = \mathscr{N}(\mathscr{M}(\hat{y}) U)$, then there exists $\alpha > 0$ such that $\alpha \hat{y} \in \Omega$.

Proof. Recall that U is the matrix whose columns form an orthonormal basis for $\mathscr{N}(X_1)$. Let W be the matrix whose columns form an orthonormal basis for the range space of X_1 and let $Q = [W \ \ U]$. Then $X_1 + \mathscr{M}(\alpha\hat{y}) \succeq 0$ for some scalar α if and only if $Q^{\mathrm{T}}(X_1 + \mathscr{M}(\alpha\hat{y}))Q \succeq 0$. But

$$Q^{\mathrm{T}}(X_1 + \mathscr{M}(\alpha\hat{y}))Q = \begin{bmatrix} \Lambda + \alpha W^{\mathrm{T}}\mathscr{M}(\hat{y})W & \alpha W^{\mathrm{T}}\mathscr{M}(\hat{y})U \\ \alpha U^{\mathrm{T}}\mathscr{M}(\hat{y})W & \alpha U^{\mathrm{T}}\mathscr{M}(\hat{y})U \end{bmatrix},$$

where Λ is the diagonal matrix of positive eigenvalues of X_1. If $U^{\mathrm{T}}\mathscr{M}(\hat{y})U \succ 0$, then $Q^{\mathrm{T}}(X_1 + \mathscr{M}(\alpha\hat{y}))Q \succeq 0$ for sufficiently small $\alpha > 0$; and hence $\alpha\hat{y} \in \Omega$ and the result follows. Thus assume that $U^{\mathrm{T}}\mathscr{M}(\hat{y})U$ is singular; and let U_1, W_1 be the matrices whose columns form an orthonormal basis for the null space and the range space of $U^{\mathrm{T}}\mathscr{M}(\hat{y})U$ respectively. Let

$$Q_1 = \begin{bmatrix} I_r & 0 & 0 \\ 0 & W_1 & U_1 \end{bmatrix},$$

where $r = \operatorname{rank} X_1$. Then

$$\begin{aligned} & Q_1^{\mathrm{T}}Q^{\mathrm{T}}(X_1 + \mathscr{M}(\alpha\hat{y}))QQ_1 \\ &\quad = \begin{bmatrix} \Lambda + \alpha W^{\mathrm{T}}\mathscr{M}(\hat{y})W & \alpha W^{\mathrm{T}}\mathscr{M}(\hat{y})UW_1 & \alpha W^{\mathrm{T}}\mathscr{M}(\hat{y})UU_1 \\ \alpha W_1^{\mathrm{T}}U^{\mathrm{T}}\mathscr{M}(\hat{y})W & \alpha\Lambda_1 & 0 \\ \alpha U_1^{\mathrm{T}}U^{\mathrm{T}}\mathscr{M}(\hat{y})W & 0 & 0 \end{bmatrix}, \end{aligned}$$

where Λ_1 is the diagonal matrix of positive eigenvalues of $U^{\mathrm{T}}\mathscr{M}(\hat{y})U$. Note that $U^{\mathrm{T}}\mathscr{M}(\hat{y})U$ has at least one positive eigenvalue since it is not equal to zero. Now $W^{\mathrm{T}}\mathscr{M}(\hat{y})UU_1 = U_1^{\mathrm{T}}U^{\mathrm{T}}\mathscr{M}(\hat{y})W = 0$ since we assumed that $\mathscr{N}(U^{\mathrm{T}}\mathscr{M}(\hat{y})U) = \mathscr{N}(\mathscr{M}(\hat{y})U)$. Furthermore, for sufficiently small positive scalar α the submatrix

$$\begin{bmatrix} \Lambda + \alpha W^{\mathrm{T}}\mathscr{M}(\hat{y})W & \alpha W^{\mathrm{T}}\mathscr{M}(\hat{y})UW_1 \\ \alpha W_1^{\mathrm{T}}U^{\mathrm{T}}\mathscr{M}(\hat{y})W & \alpha\Lambda_1 \end{bmatrix}$$

is positive definite. Thus $X_1 + \mathscr{M}(\alpha\hat{y}) \succeq 0$ and therefore $\alpha\hat{y} \in \Omega$ and the result follows. □

Lemma 4.7. *For any matrix B and any symmetric matrix A*, $\operatorname{rank} AB = \operatorname{rank} B^{\mathrm{T}}AB$ *implies* $\mathscr{N}(B^{\mathrm{T}}AB) = \mathscr{N}(AB)$.

Proof. Range $B^{\mathrm{T}}AB \subseteq$ range $B^{\mathrm{T}}A$. But $\operatorname{rank} B^{\mathrm{T}}AB = \operatorname{rank} B^{\mathrm{T}}A$ implies that $\dim(\text{range } B^{\mathrm{T}}AB) = \dim(\text{range } B^{\mathrm{T}}A)$. Thus range $B^{\mathrm{T}}AB =$ range $B^{\mathrm{T}}A$. Hence $\mathscr{N}(B^{\mathrm{T}}AB) = \mathscr{N}(AB)$. □

Proof of Theorem 3.2. Sufficiency of condition (11) follows from Corollary 4.1 and Theorem 2.1. Assume condition (12) holds, then necessity of condition (11) follows from Corollary 4.2 and Lemmas 4.6 and 4.7. □

We conclude the paper with the following two numerical examples.

5. Example 1

Let D_1 be an EDM completion of the symmetric partial matrix A where

$$D_1 = \begin{bmatrix} 0 & 5 & 10 & 10 & 5 \\ 5 & 0 & 1 & 5 & 4 \\ 10 & 1 & 0 & 4 & 5 \\ 10 & 5 & 4 & 0 & 1 \\ 5 & 4 & 5 & 1 & 0 \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} 0 & 5 & & 10 & 5 \\ 5 & 0 & 1 & 5 & \\ & 1 & 0 & 4 & 5 \\ 10 & 5 & 4 & 0 & 1 \\ 5 & & 5 & 1 & 0 \end{bmatrix}.$$

Here the free entries of A are $\{(1,3),(3,1),(2,5),(5,2)\}$. A realization P of D_1 in the plane and Gale matrix Z are given, respectively, by

$$P = \begin{bmatrix} -2 & 0 \\ 0 & 1 \\ 1 & 1 \\ 1 & -1 \\ 0 & -1 \end{bmatrix} \quad \text{and} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1/2 & -1 \\ 5/2 & 1 \\ -3 & -1 \end{bmatrix}.$$

Let

$$\Psi = \begin{bmatrix} 2 & -1 \\ -1 & 3 \end{bmatrix}.$$

Then it is easy to verify that Ψ is positive definite and $z^{1^{\mathrm{T}}}\Psi z^3 = z^{2^{\mathrm{T}}}\Psi z^5 = 0$. Hence, D_1 is unique.

Now suppose that a_{25} is specified and $a_{25} = a_{52} = 4$; and suppose that the free entries of A are now $\{(1,3),(3,1),(1,4),(4,1)\}$. Then there exists no positive definite matrix Ψ such that $z^{1^{\mathrm{T}}}\Psi z^3 = z^{1^{\mathrm{T}}}\Psi z^4 = 0$. Furthermore,

$$\left(z^1 z^{3^{\mathrm{T}}} + z^3 z^{1^{\mathrm{T}}}\right) + \left(z^1 z^{4^{\mathrm{T}}} + z^4 z^{1^{\mathrm{T}}}\right) = \begin{bmatrix} 4 & 0 \\ 0 & 0 \end{bmatrix} \succeq 0$$

and

$$(E^{13} + E^{14})Z = \begin{bmatrix} 2 & 0 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

Hence condition (13) holds since $\operatorname{rank}((z^1 z^{3^{\mathrm{T}}} + z^3 z^{1^{\mathrm{T}}}) + (z^1 z^{4^{\mathrm{T}}} + z^4 z^{1^{\mathrm{T}}})) = \operatorname{rank}(V^{\mathrm{T}}(E^{13} + E^{14})Z) = 1$. Thus in this case D_1 is not unique. In fact it is straightforward to verify that D_2 is an EDM completion of A where

$$D_2 = \begin{bmatrix} 0 & 5 & 2 & 2 & 5 \\ 5 & 0 & 1 & 5 & 4 \\ 2 & 1 & 0 & 4 & 5 \\ 2 & 5 & 4 & 0 & 1 \\ 5 & 4 & 5 & 1 & 0 \end{bmatrix}.$$

6. Example 2

This example shows that sufficiency and necessity in Theorem 3.3 need not be equivalent for $\bar{r} \geqslant 2$ if condition (13) fails to hold. Let D_1 be an EDM completion of the symmetric partial matrix A where

$$D_1 = \begin{bmatrix} 0 & 65 & 25 & 50 & 90 \\ 65 & 0 & 10 & 5 & 5 \\ 25 & 10 & 0 & 5 & 25 \\ 50 & 5 & 5 & 0 & 20 \\ 90 & 5 & 25 & 20 & 0 \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} 0 & & 25 & 50 & 90 \\ & 0 & 10 & 5 & 5 \\ 25 & 10 & 0 & & 25 \\ 50 & 5 & & 0 & 20 \\ 90 & 5 & 25 & 20 & 0 \end{bmatrix}.$$

A realization P and the Gale matrix Z corresponding to D_1 are

$$P = \begin{bmatrix} -3 & -5 \\ 1 & 2 \\ 0 & -1 \\ 2 & 0 \\ 0 & 4 \end{bmatrix}, \quad \text{and} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -3 & 0 \\ 3/2 & -1/2 \\ 1/2 & -1/2 \end{bmatrix}.$$

Note that p^2, p^4 and p^5 are collinear. In this case there does not exist a positive definite matrix Ψ such that ${z^1}^{\mathrm{T}} \Psi z^2 = {z^3}^{\mathrm{T}} \Psi z^4 = 0$ since $z^2 + 2z^4 = -z^3 = 3z^1$ even though D_1 is a unique EDM completion for A. Of course in this case condition (13) does not hold. Rank $Z^{\mathrm{T}}(E^{12} - 2/3E^{34})Z = \operatorname{rank} \begin{bmatrix} 6 & 0 \\ 0 & 0 \end{bmatrix} = 1$ while rank $V^{\mathrm{T}}(E^{12} - \frac{2}{3}E^{34})Z = 2$.

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References

[1] A.Y. Alfakih, Graph rigidity via Euclidean distance matrices, Linear Algebra Appl. 310 (2000) 149–165.
[2] A.Y. Alfakih, On rigidity and realizability of weighted graphs, Linear Algebra Appl. 325 (2001) 57–70.

[3] A.Y. Alfakih, A. Khandani, H. Wolkowicz, Solving Euclidean distance matrix completion problems via semidefinite programming, Comput. Optim. Appl. 12 (1999) 13–30.
[4] M. Bakonyi, C.R. Johnson, The Euclidean distance matrix completion problem, SIAM J. Matrix Anal. Appl. 16 (1995) 646–654.
[5] G.M. Crippen, T.F. Havel, Distance Geometry and Molecular Conformation, Wiley, New York, 1988.
[6] F. Critchley, On certain linear mappings between inner-product and squared distance matrices, Linear Algebra Appl. 105 (1988) 91–107.
[7] D. Gale, Neighboring vertices on a convex polyhedron, in: Linear Inequalities and Related System, Princeton University Press, 1956, pp. 255–263.
[8] J.C. Gower, Properties of Euclidean and non-Euclidean distance matrices, Linear Algebra Appl. 67 (1985) 81–97.
[9] R. Grone, C.R. Johnson, E.M. Sá, H. Wolkowicz, Positive definite completions of partial hermitian matrices, Linear Algebra Appl. 58 (1984) 109–124.
[10] T.L. Hayden, J. Wells, W.-M. Liu, P. Tarazaga, The cone of distance matrices, Linear Algebra Appl. 144 (1991) 153–169.
[11] B. Hendrickson, The molecule problem: Exploiting structure in global optimization, SIAM J. Optim. 5 (1995) 835–857.
[12] C.R. Johnson, Matrix completion problems: A survey, in: C.R. Johnson (Ed.), Matrix Theory and Applications, Proc. Sympos. Appl. Math., vol. 40, AMS, Providence, RI, 1990, pp. 171–198.
[13] C.R. Johnson, C. Jones, B. Kroschel, The distance matrix completion problem: Cycle completability, Linear and Multilinear Algebra 39 (1995) 195–207.
[14] M. Laurent, A tour d'horizon on positive semidefinite and Euclidean distance matrix completion problems, in: Topics in Semidefinite and Interior-Point Methods, The Fields Institute for Research in Mathematical Sciences Communications Services, vol. 18, AMS, Providence, RI, 1998, pp. 51–76.
[15] M. Laurent, Polynomial instances of the positive semidefinite and Euclidean distance matrix completion problems, SIAM J. Matrix Anal. Appl. 22 (2000) 874–894.
[16] J. De Leeuw, W. Heiser, Theory of multidimensional scaling, in: P.R. Krishnaiah, L.N. Kanal (Eds.), Handbook of Statistics, vol. 2, North-Holland, 1982, pp. 285–316.
[17] J. Moré, Z. Wu, Distance geometry optimization for protein structures, J. Global Optim. 15 (1999) 219–234.
[18] R.T. Rockafellar, Convex Analysis, Princeton University Press, 1970.
[19] I.J. Schoenberg, Remarks to Maurice Frechet's article: Sur la definition axiomatique d'une classe d'espaces vectoriels distancies applicables vectoriellement sur l'espace de Hilbert, Ann. Math. 36 (1935) 724–732.
[20] M.W. Trosset, Distance matrix completion by numerical optimization, Comput. Optim. Appl. 17 (2000) 11–22.
[21] H. Wolkowicz, R. Saigal, L. Vandenberghe (Eds.), Handbook of Semidefinite Programming. Theory, Algorithms and Applications, Kluwer Academic Publishers, Boston, MA, 2000.